

# Error Analysis of Phase-Integral Methods.

## II. Application to Wave-Penetration Problems

F. W. J. Olver

(July 1, 1965)

A study is made of the differential equation

$$d^2w/dz^2 = \{f(z) + h(z)\}w,$$

in which  $f(z)$  and  $h(z)$  are real and regular on the real axis, and  $f(z)$  has exactly two zeros there. Strict error bounds are derived for the coefficients in the formulas which connect the asymptotic solutions at  $z = +\infty$  with the asymptotic solutions at  $z = -\infty$ . Applications are made to two physical problems.

Key Words: Wave penetration, connection formulas, error bounds, potential barrier, transmission coefficient, harmonic oscillator.

### 1. Introduction and Summary

The purpose of this paper is to illustrate the theory of the preceding paper [1]<sup>1</sup> with two problems arising from the one-dimensional wave equation

$$\frac{d^2w}{dz^2} = \{f(z) + h(z)\}w. \quad (1.01)$$

In both problems the functions  $f(z)$  and  $h(z)$  are real when  $z$  is real, and in the region considered  $f(z)$  has no singularities and just two zeros, both of which are real and simple. The function  $h(z)$  is to be regarded in some sense as being small compared with  $f(z)$ , but we do not need to formulate this assumption precisely at the outset.

In the first problem (secs. 2, 3)  $f(z)$  is positive between the zeros. The object is to determine the ratio of the amplitude of an oscillatory solution at  $z = +\infty$  to the amplitudes of its components at  $z = -\infty$ .

In the second problem (secs. 4, 5)  $f(z)$  is negative between the zeros. The object here is to determine eigenconditions admitting a solution having subdominant (exponentially small) character at both  $-\infty$  and  $+\infty$ .

Both problems have been treated frequently in the literature; see the references cited in [1], and [2]–[7] given at the end of this paper. Generally, the viewpoint adopted has been that  $f(z)$  contains a multiplicative factor  $u^2$ ,  $h(z)$  is independent of  $u$ , and approximate solutions are sought which are asymptotically correct for large values of the parameter  $u$ . In the present paper, we establish explicit strict error bounds for the approximate solutions. Asymptotic properties with respect to parameters are immediate consequences of the forms of the bounds.

Two methods for solution were given in [1]. We shall concentrate on the first (Zwaan's method). As we shall see, from the standpoint of deriving error bounds this affords the simpler approach to the present problems.

### 2. The Overdense Potential Barrier

In this section we suppose that  $f(z)$  and  $h(z)$  are regular in an unbounded, simply connected complex domain  $\mathbf{D}$ , which includes the whole of the real axis, and that the only zeros of  $f(z)$  in  $\mathbf{D}$  are simple zeros at  $z = \pm a$  ( $a > 0$ ). When  $-a < z < a$ ,  $f(z)$  is positive.

<sup>1</sup> Figures in brackets indicate the literature references at the end of this paper.

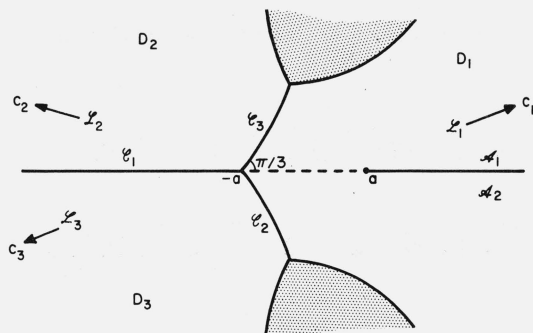


FIGURE 1. Typical principal subdomains for the overdense potential barrier.

Let us consider the turning point at  $z = -a$ . In order to apply the theory of [1], section 5, we have to exclude the other zero  $z = a$  from the domain of consideration, and we do this by introducing a cut  $\mathcal{A}$  along the real axis from  $z = a$  to  $z = +\infty$ . We shall refer to the upper and lower sides of this cut as  $\mathcal{A}_1$  and  $\mathcal{A}_2$ , respectively. As in [1], section 5, we define

$$\xi(z) = \int_{-a}^z \{f(t)\}^{1/2} dt. \quad (2.01)$$

The associated principal curves  $\mathcal{C}_j$  and subdomains  $\mathbf{D}_j$  are indicated in figure 1.  $\mathcal{C}_1$  is the part of the real axis which extends from  $-a$  to  $-\infty$ .  $\mathcal{C}_2, \mathcal{C}_3$  are conjugate curves emerging from  $-a$  at directions  $\mp \pi/3$ . They cannot intersect the real axis at any other point. We define  $\xi_j(z)$  to be the branch of  $\xi(z)$  which is continuous in  $\mathbf{D}$  cut along  $\mathcal{A}$  and  $\mathcal{C}_j$ , and has positive real part in  $\mathbf{D}_j$ . Similarly,  $g_1(z), g_2(z), g_3(z)$  are multiples of any branches of  $g(z) \equiv \{f(z)\}^{-1/4}$  which are continuous in  $\mathbf{D}$  cut along  $\mathcal{A}$  and the corresponding  $\mathcal{C}_j$ , and satisfy eq (5.08) of [1].

As in [1], let  $c_j$  be points at infinity on arbitrary  $\xi$ -progressive curves  $\mathcal{L}_j$  lying within  $\mathbf{D}_j$  such that  $|\operatorname{Re} \xi(c_j)| = \infty$ .  $\mathcal{L}_1$  is taken in the upper half-plane, and  $\mathcal{L}_2, \mathcal{L}_3$  are complex conjugates, but no boundary of  $\mathbf{D}$  may intervene between  $\mathcal{L}_2$  and  $\mathcal{L}_3$  in the neighborhood of infinity. The other assumptions we make are

(i) The variation of the function

$$F \equiv \int \left\{ \frac{h}{f^{1/2}} - \frac{1}{f^{1/4}} \frac{d^2}{dz^2} \left( \frac{1}{f^{1/4}} \right) \right\} dz \quad (2.02)$$

converges as  $z \rightarrow c_j$  along  $\mathcal{L}_j$ , and also as  $z \rightarrow \pm \infty$  along the real axis.

(ii)  $\xi$ -progressive curves can be found in  $\mathbf{D}$  linking: (a)  $c_1$  with  $c_2$ ; (b)  $c_1$  with  $c_3$ ; (c)  $c_2$  or  $c_3$  with any point of the interval  $(-\infty, -a)$ ; (d)  $c_1$  with any point of  $\mathcal{A}_1$ .

(iii)  $\epsilon_2(c_3) = 0$ ;  $\epsilon_2(z)$  and  $\epsilon_3(z) \rightarrow 0$  as  $z \rightarrow -\infty$ ;  $\epsilon_1(z) \rightarrow 0$  as  $z \rightarrow +\infty$  on  $\mathcal{A}_1$ .

(A brief discussion of the determination of  $\xi$ -progressive paths is given in the remark at the end of [1], sec. 5, and sufficient conditions for the fulfillment of (iii) are given in sec. 7 of the same paper.)

With these conditions, the fundamental connection formula ([1], sec. 5) for the solutions

$$w_j(z) = g_j(z) e^{-\xi_j(z)} \{1 + \epsilon_j(z)\} \quad (2.03)$$

of the differential eq (1.01), becomes

$$w_1(z) = e^{\pi i/3} \{1 + \epsilon_1(c_3)\} w_2(z) + e^{-\pi i/3} \{1 + \epsilon_1(c_2)\} w_3(z). \quad (2.04)$$

We fix the  $w(z)$  by specifying that  $g_1(z)$  is the branch of  $\{f(z)\}^{-1/4}$  which takes its principal value on the join of  $-a$  and  $+a$ , and interpret the branches of the two sides of (2.04) in real form, as follows.

When  $z \in \mathcal{A}_1$ , we have

$$\xi_1(z) = \alpha - i \int_a^z |f|^{1/2} dt, \quad g_1(z) = e^{\pi i/4} |f|^{-1/4}, \quad (2.05)$$

where

$$\alpha = \int_{-a}^a |f|^{1/2} dt \quad (2.06)$$

and is positive. Therefore from (2.03) and hypothesis (iii)

$$w_1(z) = e^{-\alpha} |f|^{-1/4} \{1 + o(1)\} \exp\left(i \int_a^z |f|^{1/2} dt + \frac{1}{4} \pi i\right) \quad (z \rightarrow +\infty). \quad (2.07)$$

This expression represents a *transmitted wave* ([8], p. 1100; [6]).

When  $-\infty < z < -a$ , we have

$$\xi_2(z) = i \int_z^{-a} |f|^{1/2} dt, \quad g_2(z) = e^{-\pi i/12} |f|^{-1/4}. \quad (2.08)$$

Hence

$$e^{\pi i/3} \{1 + \epsilon_1(c_3)\} w_2(z) = |f|^{-1/4} \{1 + \epsilon_1(c_3) + o(1)\} \exp\left(-i \int_z^{-a} |f|^{1/2} dt + \frac{1}{4} \pi i\right) \quad (z \rightarrow -\infty). \quad (2.09)$$

This is the *incident wave*, moving in the same direction as the transmitted wave. Similarly

$$e^{-\pi i/3} \{1 + \epsilon_1(c_2)\} w_3(z) = |f|^{-1/4} \{1 + \epsilon_1(c_2) + o(1)\} \exp\left(i \int_z^{-a} |f|^{1/2} dt - \frac{1}{4} \pi i\right) \quad (z \rightarrow -\infty). \quad (2.10)$$

This is the *reflected wave*, moving in the opposite direction to the transmitted wave.

The *transmission coefficient* <sup>2</sup>  $T$  and the *reflection coefficient*  $R$  are the squares of the limiting ratios of the wave amplitudes. Thus

$$T = e^{-2\alpha} |1 + \epsilon_1(c_3)|^{-2}, \quad (2.11)$$

$$R = |1 + \epsilon_1(c_2)|^2 |1 + \epsilon_1(c_3)|^{-2}, \quad (2.12)$$

where ([1], (5.17))

$$|\epsilon_1(c_j)| \leq \frac{1}{2} \exp \{ \mathcal{V}_{c_1, c_j}(F) \} - \frac{1}{2} \quad (j=2, 3), \quad (2.13)$$

the variations being evaluated along  $\xi$ -progressive curves.

Alternative, and sometimes more effective, formulas for  $T$  and, especially,  $R$ , can be derived with the aid of the energy-conservation eq ([8], p. 1066; [9], sec. 4.4)

$$T + R = 1. \quad (2.14)$$

<sup>2</sup> Or "tunnelling probability" [7].

(This relation may be verified analytically by means of Theorem 4 of [10] and the Wronskian property of the solutions of the differential equation.) Substitution of (2.11) and (2.12) in (2.14) yields

$$|1 + \epsilon_1(c_3)|^2 - |1 + \epsilon_1(c_2)|^2 = e^{-2\alpha}. \quad (2.15)$$

Hence

$$T = \frac{e^{-2\alpha}}{|1 + \epsilon_1(c_2)|^2 + e^{-2\alpha}}, \quad (2.16)$$

$$R = 1 - \frac{e^{-2\alpha}}{|1 + \epsilon_1(c_3)|^2} = \frac{|1 + \epsilon_1(c_2)|^2}{|1 + \epsilon_1(c_2)|^2 + e^{-2\alpha}}. \quad (2.17)$$

*Remark.* It is interesting to observe that we have not used the connection formula for the turning point at  $z = +a$ . In contrast, if the problem of this section were attacked by real-variable theory ([1], sec. 9) connection formulas at both  $-a$  and  $+a$  would have to be used, and the resulting approximate solutions of the differential equation then matched in the interval  $-a < z < a$ ; see, for example, [5, 6].<sup>3</sup> The error analysis obviously would be lengthier and lead to more complicated bounds.

### 3. Example <sup>4</sup>

Consider the modified Weber equation

$$d^2w/dz^2 = (a^2 - z^2)w \quad (a > 0). \quad (3.01)$$

We take  $f(z) = a^2 - z^2$  and  $h(z) = 0$ . Then

$$\xi(z) = \int_{-a}^z (a^2 - t^2)^{1/2} dt = \frac{1}{2} \pi a^2 - \frac{1}{2} a^2 \cos^{-1}(z/a) + \frac{1}{2} z(a^2 - z^2)^{1/2}. \quad (3.02)$$

The principal subdomains in the  $z$ -plane are shown in figure 2 (compare [12], sec. 3). The

<sup>3</sup> A real-variable method which avoids this matching has been suggested by Miller and Good [4] and by Pike [7], but it has yet to be placed on a firm mathematical foundation.

<sup>4</sup> For an account of some direct numerical calculations of transmission coefficients to high precision see [11].

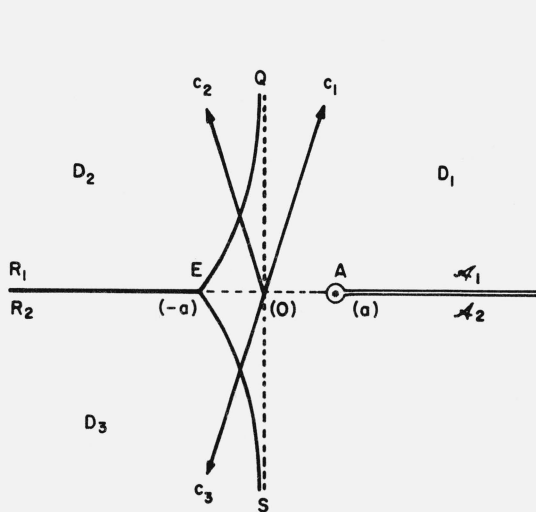


FIGURE 2.  $z$ -plane: principal subdomains.

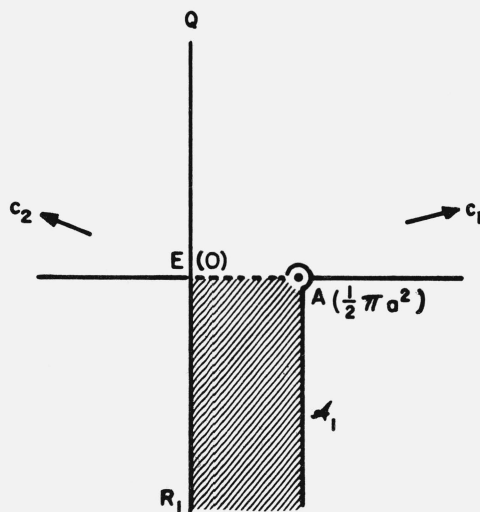


FIGURE 3.  $\xi$ -plane.

corresponding map of the upper half of the  $z$ -plane on the  $\xi_1$ -plane is indicated in figure 3; the map of the lower half is of course the image of figure 3 in the real axis.

The reference points  $c_1$ ,  $c_2$ , and  $c_3$  are taken at infinity on outward-drawn rays from the origin in the first, second, and third quadrants of the  $z$ -plane, respectively. With the aid of the  $\xi_1$ -map, we see immediately that hypotheses (i) and (ii) of section 2 are satisfied. Theorem 4 of [1] shows that hypothesis (iii) is satisfied, and also that  $\epsilon_1(c_2) = 0$ . From the definition (2.06) we have  $\alpha = \frac{1}{2} \pi a^2$ . Hence from eqs (2.16) and (2.17), we derive

$$T = \frac{e^{-\pi a^2}}{1 + e^{-\pi a^2}}, \quad R = \frac{1}{1 + e^{-\pi a^2}}. \quad (3.03)$$

These results may be verified analytically with the aid of asymptotic expansions and connection formulas for the Weber functions given, for example, in [13]. The actual expression for  $w_1(z)$  is found to be, in Miller's notation,

$$w_1(z) = 2^{-(ia^2+1)/4} a^{ia^2/2} \exp \left( -\frac{1}{2} \pi a^2 - \frac{1}{4} ia^2 - \frac{1}{2} i\varphi_2 \right) \left\{ k^{-1/2} W \left( \frac{1}{2} a^2, \sqrt{2}z \right) + ik^{1/2} W \left( \frac{1}{2} a^2, -\sqrt{2}z \right) \right\}. \quad (3.04)$$

It is noteworthy that our theory <sup>5</sup> proves sufficiently powerful to yield exact expressions for  $T$  and  $R$ . This example, however, is unique in this respect.

#### 4. The Approximate Harmonic Oscillator

The conditions assumed in this section are those stated in the opening paragraph of section 2, except that  $f(z)$  is negative when  $-a < z < a$ .

We distinguish the auxiliary functions and principal subdomains associated with the turning point at  $z = -a$  from those associated with  $z = +a$  by the addition of tildes. Thus

$$\xi(z) = \int_a^z \{f(t)\}^{1/2} dt, \quad \tilde{\xi}(z) = \int_{-a}^z \{f(t)\}^{1/2} dt. \quad (4.01)$$

Three principal curves emerge from  $-a$  and three from  $+a$ , one of which in each case is the join of  $-a$  and  $+a$ ; see figure 4. Let  $\mathbf{D}_1, \tilde{\mathbf{D}}_1$  be the principal subdomains which include the points

<sup>5</sup> This is also true of the theory of [14], section 9.1.

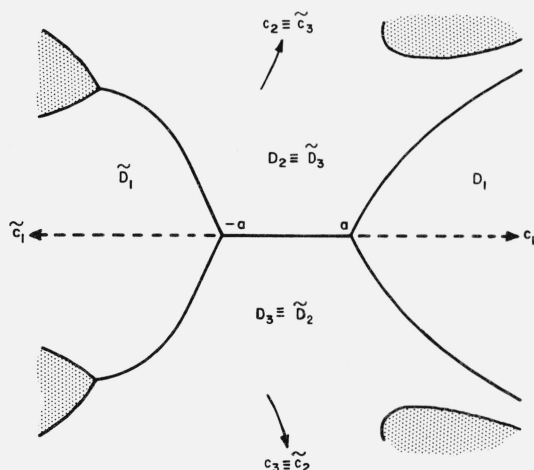


FIGURE 4. Typical principal subdomains for the approximate harmonic oscillator.

$c_1 \equiv +\infty$  and  $\bar{c}_1 \equiv -\infty$ , respectively. Then clearly  $\tilde{\mathbf{D}}_2 \equiv \mathbf{D}_3$  and  $\tilde{\mathbf{D}}_3 \equiv \mathbf{D}_2$ . We take  $c_2, c_3$  to be points at infinity on conjugate  $\xi$ -progressive curves lying within  $\mathbf{D}_2, \mathbf{D}_3$ , respectively, and  $\bar{c}_2 = c_3$ ,  $\bar{c}_3 = c_2$ . We assume that  $\xi$ -progressive curves can be found in  $\mathbf{D}$  linking  $c_2$  and  $c_3$  with  $+\infty$  and  $-\infty$ , and also with each other, and that  $|\operatorname{Re} \xi(z)| \rightarrow \infty$  as  $z$  tends to any of the  $c_j$  or  $\bar{c}_j$ .

The fundamental connection formulas for the two turning points are given by

$$\{1 + \epsilon_2(c_3)\}w_1(z) + e^{-2\pi i/3}\{1 + \epsilon_3(c_1)\}w_2(z) + e^{2\pi i/3}\{1 + \epsilon_1(c_2)\}w_3(z) = 0, \quad (4.02)$$

and

$$\{1 + \tilde{\epsilon}_2(\bar{c}_3)\}\tilde{w}_1(z) + e^{-2\pi i/3}\{1 + \tilde{\epsilon}_3(\bar{c}_1)\}\tilde{w}_2(z) + e^{2\pi i/3}\{1 + \tilde{\epsilon}_1(\bar{c}_2)\}\tilde{w}_3(z) = 0. \quad (4.03)$$

Clearly  $\tilde{w}_3(z)$  is a multiple of  $w_2(z)$ , and  $\tilde{w}_2(z)$  a multiple of  $w_3(z)$ . To fix these relationships we suppose that  $g_1(z)$  and  $\tilde{g}_1(z)$  are the branches of the function  $\{f(z)\}^{-1/4}$  which take their principal values when  $z > a$  and  $z < -a$ , respectively. We then find that if  $z \in \mathbf{D}_2$

$$\xi_2(z) = i\alpha + \tilde{\xi}_3(z), \quad g_2(z) = e^{-\pi i/6}\tilde{g}_3(z), \quad (4.04)$$

where  $\alpha$  is again defined by (2.06). Therefore

$$\tilde{w}_3(z) = e^{(\pi i/6) + i\alpha} w_2(z), \quad \tilde{\epsilon}_3(z) = \epsilon_2(z). \quad (4.05)$$

Substituting these and the corresponding results for  $\tilde{w}_2(z)$  and  $\tilde{\epsilon}_2(z)$  in (4.03), we obtain the connection formula for  $\tilde{w}_1(z)$ ,  $w_2(z)$  and  $w_3(z)$ . Elimination of  $w_3(z)$  by means of (4.02) then yields

$$w_1(z) = \left[ \frac{1 + \epsilon_1(c_3)}{1 + \epsilon_2(c_3)} + \frac{\{1 + \epsilon_1(c_2)\}\{1 + \tilde{\epsilon}_1(c_3)\}}{\{1 + \epsilon_2(c_3)\}\{1 + \tilde{\epsilon}_1(c_2)\}} \right] e^{2i\alpha} e^{\pi i/3} w_2(z) - \frac{1 + \epsilon_1(c_2)}{1 + \tilde{\epsilon}_1(c_2)} i e^{i\alpha} \tilde{w}_1(z). \quad (4.06)$$

The eigencondition or "quantization condition" is that  $w_1(z)$  be a multiple of  $\tilde{w}_1(z)$ . Accordingly, this is expressed by

$$e^{2i\alpha} = - \frac{\{1 + \epsilon_1(c_3)\}\{1 + \tilde{\epsilon}_1(c_2)\}}{\{1 + \epsilon_1(c_2)\}\{1 + \tilde{\epsilon}_1(c_3)\}}. \quad (4.07)$$

Neglecting the error terms, we obtain at once the well-known approximations  $\alpha = \frac{1}{2}\pi, \frac{3}{2}\pi, \frac{5}{2}\pi, \dots$

To assess the errors in these approximations, we write

$$\epsilon_1(c_3) = p e^{iq}, \quad \epsilon_1(c_2) = p e^{-iq}, \quad \tilde{\epsilon}_1(c_2) = \tilde{p} e^{i\tilde{q}}, \quad \tilde{\epsilon}_1(c_3) = \tilde{p} e^{-i\tilde{q}}, \quad (4.08)$$

where  $p, \tilde{p} > 0$  and  $q, \tilde{q}$  are real. Then

$$\ln \left[ \frac{\{1 + \epsilon_1(c_3)\}\{1 + \tilde{\epsilon}_1(c_2)\}}{\{1 + \epsilon_1(c_2)\}\{1 + \tilde{\epsilon}_1(c_3)\}} \right] = 2i(\omega + \tilde{\omega}), \quad (4.09)$$

where  $\omega, \tilde{\omega}$  are real, and

$$|\omega| \leq \sin^{-1} p \leq \frac{1}{2}\pi p, \quad |\tilde{\omega}| \leq \sin^{-1} \tilde{p} \leq \frac{1}{2}\pi \tilde{p}, \quad (4.10)$$

provided that  $p, \tilde{p} \leq 1$ . Hence the eigencondition is given by

$$\alpha = (n + \frac{1}{2} + \beta)\pi \quad (n = 0, 1, 2, \dots), \quad (4.11)$$

where  $\beta = (\omega + \bar{\omega})/\pi$  and is real. From (4.08), (4.10) and [1], (5.17), we obtain the desired bound

$$|\beta| \leq \frac{1}{4} \exp \{ \mathcal{V}_{\infty, c_2}(F) \} + \frac{1}{4} \exp \{ \mathcal{V}_{-\infty, c_2}(F) \} - \frac{1}{2}, \quad (4.12)$$

where  $F$  is any continuous branch of the integral defined by (2.02) above, and the variations are taken along  $\xi$ -progressive paths.

When the eigencondition is satisfied, eq (4.06) reduces to

$$w_1(z) = (-)^n \frac{1+\delta}{1+\bar{\delta}} \bar{u}_1(z), \quad (4.13)$$

where

$$|\delta| \leq \frac{1}{2} \exp \{ \mathcal{V}_{\infty, c_2}(F) \} - \frac{1}{2}, \quad |\bar{\delta}| \leq \frac{1}{2} \exp \{ \mathcal{V}_{-\infty, c_2}(F) \} - \frac{1}{2}. \quad (4.14)$$

Thus on the real axis the eigensolution is given by

$$w_1(z) = \{1 + \epsilon_1(z)\} f^{-1/4} \exp \left( - \int_a^z f^{1/2} dt \right), \quad (4.15)$$

where

$$|\epsilon_1(z)| \leq \exp \{ \mathcal{V}_{\infty, z}(F) \} - 1 \quad (z > a), \quad (4.16)$$

and

$$w_1(z) = (-)^n (1+\delta)(1+\bar{\delta})^{-1} \{1 + \bar{\epsilon}_1(z)\} f^{-1/4} \exp \left( - \int_z^{-a} f^{1/2} dt \right), \quad (4.17)$$

where

$$|\bar{\epsilon}_1(z)| \leq \exp \{ \mathcal{V}_{-\infty, z}(F) \} - 1 \quad (z < -a). \quad (4.18)$$

The fractional powers in (4.15) and (4.17) are positive, and the variations in (4.16) and (4.18) are taken along the real axis.

*Remark.* Let  $f(z)$  and  $h(z)$  be even functions of  $z$ , and assume that  $c_2, c_3$  can be taken as the points  $\pm i\infty$ . Then the bound (4.12) and eq (4.13) reduce to

$$|\beta| \leq \frac{1}{2} \exp \{ \mathcal{V}_{\infty, i\infty}(F) \} - \frac{1}{2}, \quad (4.19)$$

and

$$w_1(z) = (-)^n \bar{u}_1(z) = (-)^n w_1(-z). \quad (4.20)$$

## 5. Examples

(i) *Weber equation.*

$$d^2 w / dz^2 = (z^2 - a^2) w \quad (a > 0). \quad (5.01)$$

We take  $f(z) = z^2 - a^2$  and  $h(z) = 0$ . Then

$$\xi(z) = \int_a^z (t^2 - a^2)^{1/2} dt = \frac{1}{2} z(z^2 - a^2)^{1/2} - \frac{1}{2} a^2 \ln \{ z + (z^2 - a^2)^{1/2} \} + \frac{1}{2} a^2 \ln a. \quad (5.02)$$

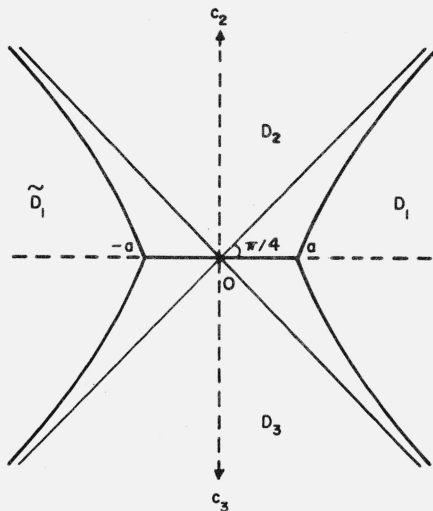


FIGURE 5. Principal subdomains for the Weber equation.

Figure 5 illustrates the principal subdomains. We take  $c_2, c_3$  to be the points  $\pm i\infty$ . From [1], theorem 4, we see that  $\epsilon_1(c_2) = \bar{\epsilon}_1(c_2) = 0$ . Hence in (4.08)  $p = \bar{p} = 0$ . Therefore  $\beta$  vanishes and  $\alpha = (n + \frac{1}{2})\pi$ , exactly.<sup>6</sup> Using (2.06), we see that this implies  $a^2 = 2n + 1$ . The eigensolution of course obeys (4.20). These results accord with the known analytical properties of the Weber functions [13].

(ii) *Large parameter.* Let  $f(z) = u^2 f_0(z)$ , where  $u$  is a large positive parameter, and the functions  $f_0(z)$  and  $h(z)$  are independent of  $u$  (though this restriction could be eased without significantly affecting the following analysis). Then

$$\alpha = u\alpha_0, \quad F(z) = F_0(z)/u, \quad (5.03)$$

where

$$\alpha_0 = \int_{-a}^a |f_0|^{1/2} dt, \quad F_0(z) = \int \left\{ \frac{h}{f_0^{1/2}} - \frac{1}{f_0^{1/4}} \frac{d^2}{dz^2} \left( \frac{1}{f_0^{1/4}} \right) \right\} dz, \quad (5.04)$$

and are independent of  $u$ . Write

$$\chi(u) \equiv \frac{1}{4} \exp \{u^{-1} \psi_{-\infty, c_2}(F_0)\} + \frac{1}{4} \exp \{u^{-1} \psi_{-\infty, c_2}(F_0)\} - \frac{1}{2}. \quad (5.05)$$

Then the eigencondition (4.11) is expressed by the following equation for  $u$ :

$$\psi(u) \equiv u\alpha_0 - (n + \frac{1}{2})\pi - \pi\beta(u) = 0, \quad (5.06)$$

in which

$$|\beta(u)| \leq \chi(u). \quad (5.07)$$

For large  $u$ ,  $\chi(u) = O(u^{-1})$ . Therefore for large values of the positive integer  $n$

$$u = \alpha_0^{-1}(n + \frac{1}{2})\pi + O(n^{-1}). \quad (5.08)$$

<sup>6</sup> Compare also [14], page 109.



In order to determine precise bounds for the  $O$  term in the last equation, consider the function  $\chi(u)$ . This tends to infinity as  $u \rightarrow 0$ , and to zero as  $u \rightarrow \infty$ , and is monotonic strictly decreasing when  $u$  is positive. Let  $u_0$  be the root of  $\chi(u_0) = \frac{1}{2}$ . Then provided that  $n\pi/\alpha_0 > u_0$ , we have from (5.06) and (5.07)

$$\psi(n\pi/\alpha_0) = -\frac{1}{2}\pi - \pi\beta(n\pi/\alpha_0) < 0, \quad (5.09)$$

and

$$\psi\{(n+1)\pi/\alpha_0\} = \frac{1}{2}\pi - \pi\beta\{(n+1)\pi/\alpha_0\} > 0. \quad (5.10)$$

Therefore at least one eigenvalue exists in the interval  $n\pi/\alpha_0 < u < (n+1)\pi/\alpha_0$ . To delimit it in a shorter interval, let

$$u = (n + \frac{1}{2} + v)\pi/\alpha_0, \quad (5.11)$$

where  $|v| < \frac{1}{2}$ . Then substituting in (5.06), we obtain

$$v = \beta\{(n + \frac{1}{2} + v)\pi/\alpha_0\}. \quad (5.12)$$

Hence  $|v| < \chi(n\pi/\alpha_0)$ , that is,

$$|v| < \frac{1}{4} \exp \left\{ \frac{\alpha_0}{n\pi} \mathcal{V}_{-\infty, c_2}(F_0) \right\} + \frac{1}{4} \exp \left\{ \frac{\alpha_0}{n\pi} \mathcal{V}_{-\infty, c_2}(F_0) \right\} - \frac{1}{2}. \quad (5.13)$$

Relations (5.11) and (5.13) constitute the precise form of the eigencondition (5.08), and are valid when  $n > \alpha_0 u_0/\pi$ . The eigensolution satisfies (4.13), where

$$|\delta| \leq \frac{1}{2} \exp \left\{ \frac{\alpha_0}{n\pi} \mathcal{V}_{-\infty, c_2}(F_0) \right\} - \frac{1}{2}, \quad |\bar{\delta}| \leq \frac{1}{2} \exp \left\{ \frac{\alpha_0}{n\pi} \mathcal{V}_{-\infty, c_2}(F_0) \right\} - \frac{1}{2}. \quad (5.14)$$

The above proof shows that there is at least one eigenvalue (5.11) which satisfies (5.13). In order to establish that there is *exactly* one eigenvalue of this form, we need to investigate the sign of the derivative  $\beta'(u)$  in the interval considered.<sup>7</sup> This takes us back to fundamentals. We have to consider the Liouville-Green approximate solutions of the differential equation

$$d^2w/dz^2 = \{u^2 + f(z)\}w \quad (5.15)$$

(compare [1], sec. 2) as functions of  $u$ , and seek bounds for the  $u$ -derivatives of their error terms. The analysis is somewhat lengthy, and we record only the result:

Let

$$X(u) = \frac{le^l}{3-e^l} \frac{1+\kappa}{u} + \frac{\bar{l}e^{\bar{l}}}{3-e^{\bar{l}}} \frac{1+\bar{\kappa}}{u} - \alpha_0, \quad (5.16)$$

where

$$l = u^{-1} \mathcal{V}_{-\infty, c_2}(F_0), \quad \bar{l} = u^{-1} \mathcal{V}_{-\infty, c_2}(F_0), \quad (5.17)$$

$$\kappa = (2e \cos \gamma)^{-1}, \quad \bar{\kappa} = (2e \cos \bar{\gamma})^{-1}, \quad (5.18)$$

<sup>7</sup> An alternative, but apparently no easier, approach would be to consider complex values of  $u$  and apply Rouché's theorem.

and  $\gamma$ ,  $\tilde{\gamma}$  are the maximum angles of slope with the real  $\xi$ -axis of the  $\xi$ -maps of the progressive paths linking  $\infty$  to  $c_2$ , and  $-\infty$  to  $c_2$ , respectively ( $|\gamma|, |\tilde{\gamma}| < \frac{1}{2}\pi$ ). Then exactly one eigenvalue satisfies (5.11) and (5.13), provided that  $n \geq \alpha_0 u_1/\pi$  where  $u_1$  is the largest positive zero of  $X(u)$ .

Some simplification can be effected by using upper bounds for the zeros of  $\chi(u) - \frac{1}{2}$  and  $X(u)$ . In this way we may verify that both of the conditions  $n > \alpha_0 u_0/\pi$  and  $n \geq \alpha_0 u_1/\pi$  are certainly fulfilled if  $n$  exceeds each of the three quantities

$$\frac{\alpha_0 \mathcal{V}_{x, c_2}(F_0)}{\pi \ln 2}, \quad \frac{\alpha_0 \mathcal{V}_{-x, c_2}(F_0)}{\pi \ln 2}, \quad \frac{2 \ln 2}{\pi} (2 + \kappa + \bar{\kappa}). \quad (5.19)$$

The author acknowledges helpful criticisms of the draft of this paper by Drs. J. Heading and L. Maximon.

The work described above has been supported by the U.S. Army Research Office, Durham, N. Carolina (Project No. 4238-M).

## 6. References

- [1] Olver F. W. J., Error analysis of phase-integral methods. I. General theory for simple turning points, J. Res. NBS **69B**, No. 4, 271-290 (1965).
- [2] Dunham, J. L., The Wentzel-Brillouin-Kramers method of solving the wave equation, Phys. Rev. **41**, 713-720 (1932).
- [3] Birkhoff, G. D., Quantum mechanics and asymptotic series. Bull. Amer. Math. Soc. **39**, 681-700 (1933).
- [4] Miller, S. C., and Good, R. H., A WKB-type approximation to the Schrödinger equation, Phys. Rev. **91**, 174-179 (1953).
- [5] Jeffreys, H., On the use of asymptotic approximations of Green's type when the coefficient has zeros, Proc. Camb. Phil. Soc. **52**, 61-66 (1956).
- [6] McLeod, J. B., The determination of the transmission coefficient, Quart. J. Math. Oxford (2) **12**, 153-158 (1961).
- [7] Pike, E. R., On the related-equation method of asymptotic approximation II. Direct solutions of wave-penetration problems, Quart. J. Mech. Appl. Math. **17**, 369-379 (1964).
- [8] Morse, P. M., and Feshbach, H., Methods of Theoretical Physics, Pt 2 (McGraw-Hill Book Co., Inc., New York, N.Y., 1953).
- [9] Heading, J., An Introduction to Phase-Integral Methods (John Wiley & Sons, Inc., New York, N.Y., 1962).
- [10] Olver, F. W. J., Error bounds for the Liouville-Green (or WKB) approximation, Proc. Camb. Phil. Soc. **57**, 790-810 (1961).
- [11] Jamet, P., Calcul exact du coefficient de transmission d'une barrière de potentiel: étude de l'erreur de l'approximation BKW (in press).
- [12] Olver, F. W. J., Uniform asymptotic expansions for Weber parabolic cylinder functions of large orders, J. Res. NBS **63B** (Math. and Math. Phys.), No. 2, 131-169 (1959).
- [13] Miller, J. C. P., Tables of Weber parabolic cylinder functions (Her Majesty's Stationery Office, London, 1955).
- [14] Fröman, N., and Fröman, P. O., JWKB approximation - Contributions to the theory (North-Holland Publishing Co., Amsterdam, 1965).

(Paper 69B4-158)